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Proton-neutron pairing energies in $N = Z$ nuclei at finite temperature

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The thermal behavior of isoscalar ($\tau = 0$) and isovector ($\tau = 1$) proton-neutron (*pn*) pairing energies at finite temperature is investigated with shell-model calculations. These *pn* pairing energies can be estimated by double differences of "thermal" energies that are extended from the double differences of binding energies as indicators of *pn* pairing energies at zero temperature. We found that the delicate balance between isoscalar and isovector *pn* pairing energies at zero temperature disappears at a finite temperature. When the temperature rises, while the isovector *pn* pairing energy decreases, the isoscalar *pn* pairing energy rather increases. We also discuss the symmetry energy at finite temperature.

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The proton-neutron (*pn*) pairing energies have become one of hot topics in the study of the nuclear structure for proton-rich nuclei. In particular, interest is increasing in studying isovector ($\tau = 1$) and isoscalar ($\tau = 0$) *pn* pairing energies in medium mass $N = Z$ nuclei produced at radioactive nuclear beam facilities. The study of *pn* pairing energies is also important in the astrophysical context. These nuclei lie along the explosive *rp*-process nucleosynthesis path, and nuclear properties such as masses, half-lives, and isomers have a strong influence on modeling the *rp* process and identifying possible nucleosynthesis sites. Odd-odd $N = Z$ nuclei are an ideal experimental laboratory for the study of *pn* pairing energies. It is well known that the lowest $\tau = 0$ and $\tau = 1$ states compete for the ground state, changing the sign of the energy difference $E_{\tau=1} - E_{\tau=0}$ in odd-odd $N = Z$ nuclei, whereas all even-even $N = Z$ nuclei have $\tau = 0$ ground states. Several authors [1–7] have already pointed out that this degeneracy in odd-odd $N = Z$ nuclei reflects the delicate balance between the symmetry energy and the like-nucleon neutron-neutron (*nn*) [or proton-proton (*pp*)] pairing energy. On the other hand, it has recently been shown that this degeneracy is attributed to competition between the isoscalar and isovector pairing energies [8–10].

It has been recently reported [11,12] that the canonical heat capacities extracted from observed level densities in ^{162}Dy, ^{166}Er, and ^{172}Yb display the *S* shape with a peak around $T \approx 0.5$ MeV, which is interpreted as the breaking of like-nucleon $J = 0$ pairs because the BCS critical temperature corresponds to $T_c \approx 0.57\Delta_n(T = 0) \approx 0.5$ MeV, in which the like-nucleon pairing gap $\Delta_n(T = 0)$ is calculated at zero temperature by the BCS theory. Thus it seems that the *S* shape is a signature of pairing transition at the critical temperature. For a finite Fermi system like a nucleus, however, because the nuclear radius is much smaller than the coherence length of the Cooper pair, statistical fluctuations beyond the mean field in the BCS theory become large. The fluctuations smooth out the sharp phase transition, and then the like-nucleon pairing gap Δ_n does not quickly become zero at the BCS critical temperature but decreases with increasing temperature. There are many approaches to treat the fluctuations beyond the mean field. The shell-model calculation can take into account the large fluctuations beyond the mean field. Recently the shell-model Monte Carlo (SMMC) calculation [13,14], in which the $fp + g_{9/2}$ shell was used, has been performed in the even- and odd-mass Fe isotopes.

We recently proposed [15] a "thermal" odd-even-mass difference to estimate the like-nucleon pairing energy at a finite temperature and showed in the spherical shell-model calculations that the drastic suppression of like-nucleon pairing energy that is due to finite temperature brings about the *S* shape in the heat capacity arround the temperature $T_c \approx 0.57\Delta_n$ ($T = 0$) MeV. In this rapid communication, we study the *pn* pairing energies at finite temperature in odd-odd $N = Z$ nuclei. Does pairing transition that is due to the breaking of *pn* pairs take place when the temperature increases? It is now interesting to investigate the thermal behavior of the *pn* pairing energies in $N = Z$ nuclei.

We start from the double difference of binding energies [16–18] defined as

$$\Delta^{\tau}_{pn}(Z,N) = \tfrac{1}{2}[B(Z,N)^{\tau} - B(Z,N-1) - B(Z-1,N) + B(Z-1,N-1)], \quad (1)$$

where $B(Z,N)$ is the binding energy. The indicator $\Delta^{\tau=1}_{pn}$ gives the $\tau = 1$ *pn* pairing gap in $N = Z$ nuclei. The $\Delta^{\tau=0}_{pn}$ can be regarded as the $\tau = 0$ *pn* pairing gap as well. Figure 1(a) shows the $\tau = 0$ and $\tau = 1$ *pn* pairing gaps estimated from the double differences of experimental binding energies [Eq.(1)] in odd-odd $N = Z$ nuclei with $A = 18 - 58$. The $\tau = 0$ *pn* energy is somewhat larger than the $\tau = 1$ *pn* energy in the *sd* shell nuclei and vice versa in the *pf* shell nuclei. Over a wide range of odd-odd $N = Z$ nuclei, however, basically Fig. 1 shows almost the same magnitude of the $\tau = 0$ and $\tau = 1$ *pn* pairing gaps. We carried out shell-model calculations by using isospin-invariant interactions such as the unified *sd* (USD) interaction [19] for odd-odd $N = Z$ nuclei in *sd* shell and GXPF1 interactions [20] for ^{42}Sc, ^{46}V, and ^{50}Mn in the *fp* shell. On the mean-field level the ratio between the strengths of *pp*, *nn*, and *pn* pair fields is given by the orientation of the pair field. The relative strengths of three types of pair fields becomes definite only when isospin symmetry is restored.

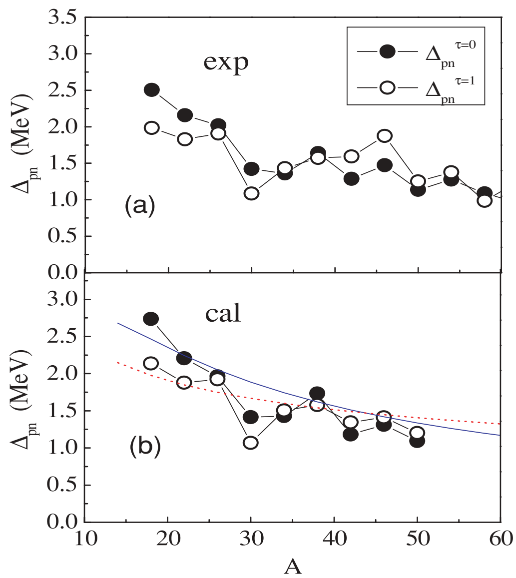

FIG. 1. (Color online) $\tau = 0$ and $\tau = 1$ *pn* pairing gaps estimated from double differences of binding energies for odd-odd $N = Z$ nuclei: (a) experimental ones; (b) those of shell-model calculations. The solid and dotted curves show $122.25(1 - 1.67A^{-1/3})/A$ and $5.18A^{-1/3}$, respectively.

Note that the shell-model calculations with isospin invariance show $\Delta_{pp}^{\tau=1} = \Delta_{nn}^{\tau=1} = \Delta_{pn}^{\tau=1}$ in odd-odd $N = Z$ nuclei.

In Fig. 1(b), we can see that the shell-model results reproduce well the experimental *pn* pairing gaps and describe the characteristic behavior in Fig. 1(a). The *pn* pairing gaps are closely related to the energy difference $B(Z,N)^{\tau=1} - B(Z,N)^{\tau=0}$ between the lowest $\tau = 0$ and $\tau = 1$ states in odd-odd $N = Z$ nuclei, because the energy difference satisfies the following identity [9]:

$$B(Z,N)^{\tau=1} - B(Z,N)^{\tau=0} = 2\left(\Delta_{pn}^{\tau=0} - \Delta_{pn}^{\tau=1}\right). \quad (2)$$

Odd-odd $N = Z$ nuclei with $A < 40$ have ground states with $\tau = 0$, $J > 0$, except for ^{34}Cl, whereas the ground states of odd-odd $N = Z$ nuclei with $40 < A < 74$ are $\tau = 1$ and $J = 0$, except for ^{58}Cu. Several authors [1–3,5–7] discussed that this degeneracy is attributed to the delicate balance between the symmetry energy $a(A)\tau(\tau + 1)/A$ and pairing gap Δ and that the energy difference $\delta B = B(Z,N)^{\tau=1} - B(Z,N)^{\tau=0}$ is expressed as $\delta B = 2[a(A)/A - \Delta]$. However, if we employ the symmetry-energy coefficient $a(A) = 134.4(1 - 1.52A^{-1/3})$ and pairing gap $\Delta = 5.18A^{-1/3}$ of the Duflo and Zuker mass formula [21], the energy difference δB becomes larger than the experimental value. As suggested in our previous paper, the isoscalar pairing gap $\Delta_{pn}^{\tau=0}$ is approximately written as $122.25(1 - 1.67A^{-1/3})/A$ and the isovector one, $\Delta_{pn}^{\tau=1}$, is equal to the like-nucleon *nn* pairing gap $\Delta_n \approx 5.18A^{-1/3}$. These two curves are shown in Fig. 1(b) for comparison. Because $\delta B = 2(\Delta_{pn}^{\tau=1} - \Delta_{pn}^{\tau=0})$, the degeneracy between the lowest $\tau = 0$ and $\tau = 1$ states in odd-odd $N = Z$ nuclei comes from the delicate balance between the isoscalar and isovector *pn* pairing energies.

Let us next describe the *pn* pairing gaps at finite temperature. We introduce the canonical partition function defined by

$$Z(T) = \mathrm{Tr}(e^{-H/T}) = \sum_{i=0}^{\infty} e^{-E_i/T}, \quad (3)$$

where E_i is the energy of the ith eigenstate with degeneracies based on symmetries for the Hamiltonian H of a system. All the eigenvalues E_i are obtained from the solution of the eigenvalue equations $H\Psi_i = E_i\Psi_i$. Then the partition function in the canonical ensemble is calculated from Eq. (3), and any thermodynamical quantities $O(T)$ can be evaluated from

$$O(T) = \langle O \rangle = \mathrm{Tr}(Oe^{-H/T})/Z(T), \quad (4)$$

where $\langle O \rangle$ is the average value of operator O over the range of eigenstates. For instance, the thermal energy is expressed as

$$E(Z,N,T) = \langle H \rangle = \sum_{i=0}^{\infty} E_i e^{-E_i/T}/Z(T). \quad (5)$$

The heat capacity is then given by

$$C(Z,N,T) = \frac{\partial E(Z,N,T)}{\partial T}. \quad (6)$$

We now introduce the following double difference of thermal enegies $E(Z,N,T)$ analogous to Eq. (1) as an indicator of *pn* pairing energies:

$$\Delta_{pn}^{\tau}(Z,N,T) = \tfrac{1}{2}[E(Z,N,T)^{\tau} - E(Z,N-1,T) - E(Z-1,N,T) + E(Z-1,N-1,T)]. \quad (7)$$

The double differences of binding energies at zero temperature in Eq. (1) are known theoretically and experimentally as important quantities in the evaluation of the *pn* pairing energies in a nucleus [16–18]. The double differences of thermal energies in Eq. (7) are also indicators of the *pn* pairing energies and can be regarded as the *pn* pairing gaps at finite temperature.

Let us evaluate the double difference of thermal energies [Eq. (7)] for $N = Z$ *sd* shell nuclei. We make numerical calculations in two steps. First, we carry out the exact shell-model calculations in the *sd* shell by using the USD interaction [19] and calculate the correlated thermal energy $E_{v,\mathrm{tr}}$ from Eq. (5). Second, we extend the model space to a larger one ($sd + fp + s_{1/2}d_{5/2}$) in order to display the double difference of thermal energies in a broader range of temperature by using an independent-particle approximation [14]. We obtain the single-particle energies of the extended space by diagonalizing the Woods-Saxon potential with the spin-orbit interaction [22], in which the harmonic-oscillator eigenfunctions are used. The Woods-Saxon parameters are chosen so as to reproduce the single-particle energies estimated from ^{17}O, because it is necessary to reasonably extrapolate the single-particle energies of the *sd* shell to those of the larger space. In this way, we combine the correlated thermal energy $E_{v,\mathrm{tr}}$ in the truncated space with the thermal energy E_{sp} calculated with the independent-particle approximation in the larger space. The thermal energy which takes account of the

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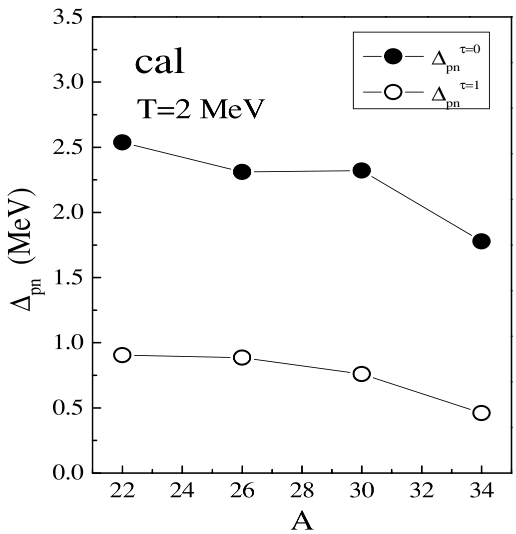

FIG. 2. Calculated thermal pn pairing gaps for odd-odd $N = Z$ nuclei at temperature $T = 2.0$ MeV. The solid circles denote the $\tau = 0$ pn pairing gap, and the open circles denote the $\tau = 1$ pn pairing gap.

interaction effects in the *sd* shell is estimated as follows [14]:

$$E = E_{v,\mathrm{tr}} + E_{\mathrm{sp}} - E_{\mathrm{sp,tr}}, \tag{8}$$

where $E_{\mathrm{sp,tr}}$ is the thermal energy of the *sd* shell within the independent-particle approximation. We now obtain the double difference of thermal energies Δ^{τ}_{pn} by substituting E of Eq. (8) for $E(Z,N,T)$ in Eq. (7).

Figure 2 shows the calculated thermal pn pairing gaps for odd-odd $N = Z$ nuclei, ^{22}Na, ^{26}Al, ^{30}P, and ^{34}Cl at temperature $T = 2.0$ MeV. The $\tau = 1$ and $\tau = 0$ pn pairing gaps are largely separated at $T = 2.0$ MeV. Comparing Fig. 2 with Fig. 1(b), we note that the $\tau = 1$ pn pairing gap decreases but the $\tau = 0$ pn pairing gap keeps the magnitude from zero temperature to high temperature.

Figure 3 shows the variation of the thermal pn pairing gaps depending on temperature T for ^{22}Na, ^{26}Al, ^{30}P, and ^{34}Cl. In all graphs, we can see an increase in the $\tau = 0$ pn pairing gap and a decrease in the $\tau = 1$ pn pairing gap. As already mentioned, at zero temperature the $\tau = 0$ and $\tau = 1$ pn pairing gaps are almost the same and the lowest $\tau = 0$ and $\tau = 1$ states are degenerate. As the temperature increases, the $\tau = 1$ pn pairing gap decreases and the $\tau = 0$ one rather increases. Thus we know that the $\tau = 0$ pairing energy becomes dominant at high temperatures.

It would be valuable to discuss the symmetry energy $\sim 4a_{\mathrm{sym}}(T)\tau(\tau + 1)/A$ at finite temperature because it is closely related to the $\tau = 0$ pairing energy. In our previous paper [18], we suggested that the dominant part of the symmetry energy comes from the $\tau = 0$ pairing energy part in the shell-model interaction energy. For the application of the symmetry energy in core-collapse supernova simulations, Donati *et al.* [23] pointed out the possibility that the symmetry-energy coefficient a_{sym} at finite temperature has been estimated to be somewhat larger than that of stable nuclei at zero temperature. The increase ($\sim$3%) of the symmetry energy

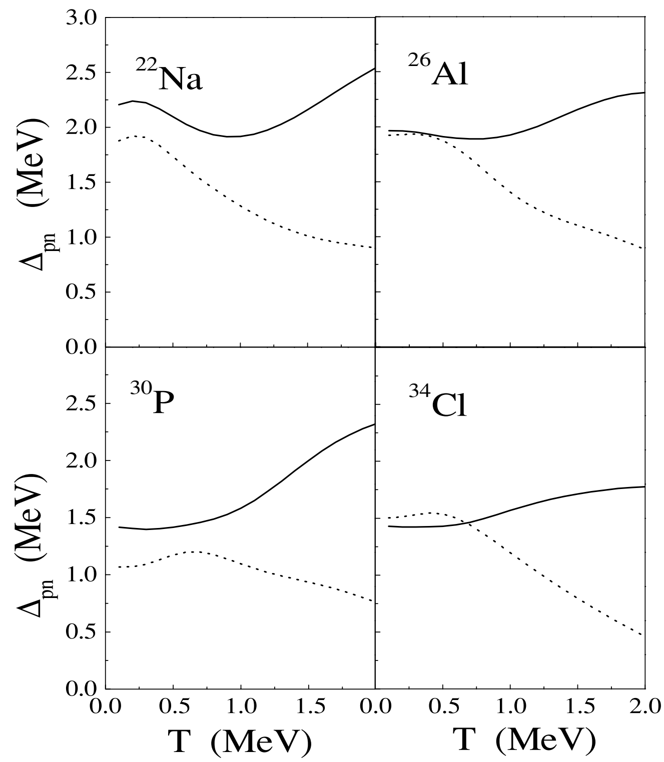

FIG. 3. Calculated thermal pn pairing gaps for odd-odd $N = Z$ nuclei as a function of temperature. The solid line denotes the $\tau = 0$ pn pairing gap, and the dotted line the $\tau = 1$ pn pairing gap.

between $T = 0.0$ and $T = 1.0$ MeV after the correction in the SMMC calculations is implemented is smaller than that ($\sim$8%) of the quasiparticle random-phase approximation with temperature [24]. We now calculate the temperature dependence of the symmetry energy by using the shell-model calculations. We estimate the symmetry-energy coefficient from the thermal energy $E(Z,N,T)^{\tau}$ with isospin τ and temperature T obtained in the shell-model calculations as follows:

$$a_{\mathrm{sym}}(T) = \frac{E(Z,N,T)^{\tau} - E(Z,N,T)^{\tau'}}{\tau(\tau + 1) - \tau'(\tau' + 1)} A, \tag{9}$$

where τ and τ' are different isospins for isobaric nuclei with same mass number A. At zero temperature, the calculated symmetry-energy coefficient $a_{\mathrm{sym}}(T = 0) \sim 16$ MeV for $A = 24$ is in good agreement with the value determined from experimental masses and with the empirical value of the Duflo and Zuker mass formula.

Figure 4 shows the symmetry-energy coefficient a_{sym} as a function of the temperature for even-even $N \approx Z$ nuclei with mass numbers $A = 20$, 24, and 28, in which several isobaric pairs of $N \approx Z$ nuclei such as (^{20}Ne,^{20}O), (^{24}Mg,^{24}Ne), and (^{28}Si,^{28}Mg) are chosen. This figure shows that the symmetry-energy coefficients increase with increasing temperature in these three cases. Moreover, we can see that the symmetry-energy coefficient depends on the mass A that is empirically fitted by adding the surface contribution with the $A^{-1/3}$ dependence at zero temperature. This mass dependence

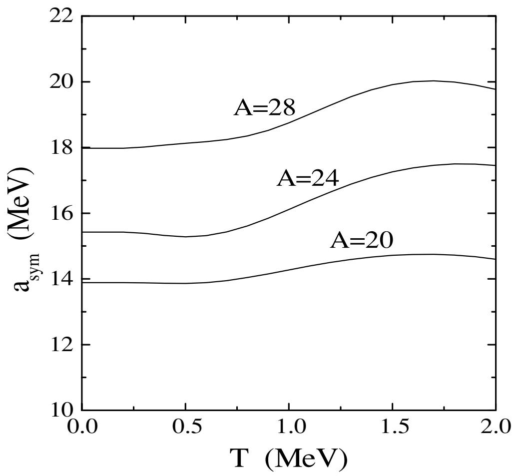

FIG. 4. Symmetry-energy coefficient $a_{\rm sym}$ as a function of temperature for $N \approx Z$ nuclei with mass numbers $A = 20$, 24, and 28.

appears in the $\tau = 0$ *pn* pairing gap estimated from the double difference of binding energies in Fig. 1(b). Figure 4 also suggests that the mass dependence changes as temperature increases. To see the temperature dependence of the symmetry-energy coefficient, we define the relative change of the symmetry-energy coefficient with respect to temperature as

$$\delta a_{\rm sym}(T) = \frac{a_{\rm sym}(T) - a_{\rm sym}(T = 0)}{a_{\rm sym}(T = 0)}. \qquad (10)$$

Averaging the $\delta a_{\rm sym}(T)$ at $T = 1.0$ MeV over various pairs of nuclei, we obtain an increase of ∼4%. This is in agreement with the SMMC result ∼3% obtained after the correction is implemented. We used here the form of symmetry energy $\tau(\tau + 1)$, which is motivated by the charge independence of the nuclear force. However, as a phenomenological parametrization, the isospin dependence $\tau(\tau + \alpha)$ with $\alpha \neq 1$ is also possible, where the linear term in τ is the so-called Wigner term. Recently, empirical fitting to the Wigner term gave $\alpha = 1.25$ in the vicinity of the $N = Z$ line [2,25]. However, the symmetry-energy coefficient is little affected when $\tau(\tau + 1)$ is replaced with $\tau(\tau + 1.25)$. Moreover, by definition, the relative change of the symmetry-energy coefficient $\delta a_{\rm sym}(T)$ does not change by this replacement.

In conclusion, we investigated the $\tau = 0$ and $\tau = 1$ *pn* pairing energies at finite temperature by using the shell-model calculations. The *pn* pairing gaps at finite temperature were estimated from the double differences of thermal energies defined by Eq. (7), which is analogous to the double differences of binding energies as indicators of the *pn* pairing energies at zero temperature. It was shown that as the temperature increases the isoscalar *pn* pairing energy increases, whereas the isovector *pn* pairing energy decreases. Almost the same *pn* pairing gaps of stable $N = Z$ nuclei at zero temperature are separated with increasing temperature. We also studied the temperature dependence of the symmetry energy in $N \approx Z$ nuclei. The symmetry energy coefficients increase with increasing temperature. The increase of the calculated symmtery-energy coefficient between $T = 0.0$ and $T = 1.0$ MeV is in good agreement with that of the SMMC calculations. We suggest that the *pn* pairing energies can be estimated by use of Eqs. (5) and (7) from the measured level densities of nuclei. We expect that the *pn* pairing energies play an important role in the astrophysics.

[1] P. Vogel, Nucl. Phys. **A662**, 148 (2000).
[2] J. Jänecke, Nucl. Phys. **73**, 97 (1965).
[3] N. Zeldes and S. Liran, Phys. Lett. **B62**, 12 (1976).
[4] G. Martinez-Pinedo, K. Langanke, and P. Vogel, Nucl. Phys. **A651**, 379 (1999).
[5] A. O. Macchiavelli, P. Fallon, R. M. Clark, M. Cromaz, M. A. Deleplanque, R. M. Diamond, G. J. Lane, I. Y. Lee, F. S. Stephens, C. E. Svensson, K. Vetter, and D. Ward, Phys. Rev. C **61**, 041303(R) (2000); Phys. Lett. **B480**, 1 (2000).
[6] J. Jänecke, T. W. O'Donnell, and V. I. Goldanskii, Phys. Rev. C **66**, 024327 (2002).
[7] S. Frauendorf and J. Sheikh, Nucl. Phys. **A645**, 509 (1999).
[8] W. Satula and R. Wyss, Phys. Rev. Lett. **86**, 4488 (2001); **87**, 052504 (2001).
[9] K. Kaneko and M. Hasegawa, Phys. Rev. C **69**, 061302(R) (2004).
[10] M. Hasegawa and K. Kaneko, Nucl. Phys. **A748**, 393 (2005).
[11] A. Schiller, A. Bjerve, M. Guttormsen, M. Hjorth-Jensen, F. Ingebretsen, E. Melby, S. Messelt, J. Rekstad, S. Siem, and S. W. Ødegard, Phys. Rev. C **63**, 021306(R) (2001).
[12] E. Melby, L. Bergholt, M. Guttormsen, M. Hjorth-Jensen, F. Ingebretsen, S. Messelt, J. Rekstad, A. Schiller, S. Siem, and S. W. Ødegard, Phys. Rev. Lett. **83**, 3150 (1999).
[13] S. Liu and Y. Alhassid, Phys. Rev. Lett. **87**, 022501 (2001).
[14] Y. Alhassid, G. F. Bertsch, and L. Fang, Phys. Rev. C **68**, 044322 (2003).
[15] K. Kaneko and M. Hasegawa, Nucl. Phys. **A740**, 95 (2004).
[16] J. Jänecke and H. Brehrens, Phys. Rev. C **9**, 1276 (1974).
[17] A. S. Jensen, P. G. Hansen, and B. Jonson, Nucl. Phys. **A431**, 393 (1984).
[18] K. Kaneko and M. Hasegawa, Phys. Rev. C **60**, 024301 (1999); Prog. Theor. Phys. **106**, 1179 (2001).
[19] B. A. Brown and B. H. Wildenthal, Annu. Rev. Nucl. Part. Sci. **38**, 29 (1988).
[20] M. Honma, T. Otsuka, B. A. Brown, and T. Mizusaki, Phys. Rev. C **69**, 034335 (2004).
[21] J. Duflo and A. P. Zuker, Phys. Rev. C **52**, R23 (1995).
[22] S. Cwiok, J. Dudek, W. Nazarewicz, J. Skalski, and T. Werner, Comput. Phys. Commun. **46**, 379 (1987).
[23] P. Donati, P. M. Pizzochero, P. F. Bortignon, and R. A. Broglia, Phys. Rev. Lett. **72**, 2835 (1994).
[24] D. J. Dean, K. Langanke, and J. M. Sampaio, Phys. Rev. C **66**, 045802 (2002).
[25] S. Glowacz, W. Satula, and R. A. Wyss, Eur. Phys. J. A **19**, 33 (2004).